

## ABSTRACT

A method of simulating multibody dynamics of a molecular system so as to produce output data representative of a time evolution of the molecular system includes providing a set of equations for characterizing multibody dynamics of the molecular system. The set of equations is constrained by a constraining equation. The method further includes providing an integrator for integrating the set of equations. The integrator is tailored for the set of equations so as to satisfy the constraining equation. The method further includes applying the integrator to the set of equations over a time step, so as to produce output data representative of the time evolution of the molecular system relative to the time step.